# Chapter 6

# Physics and Chemistry

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## 6.1 Introduction

Four sets of experiments are described that use either the reduced gravity or the large pumping speeds and vast reduced pressure domains available on or outside the station. The scientific rationale for each of the four sets is contained in the individual descriptions that follow below. In addition, we propose an analysis facility with surface analysis instrumentation that in our view would be crucial onboard the Space Station. Although our suggestions by way of experiments are quite specific, we recognise that with a ten year lead-time many details will necessarily change in the interim and our specificity is to be regarded only as an attempt to give our proposals substance, realizing that what we are proposing are classes of experiments.

We also realise that there is considerable overlap with the science and most certainly with the technology required by other disciplines. For example, experiments regarding the formation and stability of planetary rings clearly overlaps with the two projects involving assemblies of inelastic frictional particles of this section. Likewise, the light-scattering technology needed in some of the experiments proposed in the astrophysics chapter will be essential in ours.

## 6.2 Suggested Experiments for Space Station

### 6.2.1 Rheology of Assemblies of Inelastic, Frictional Particles

The rheologic properties of granular solids is important in a wide variety of scientific as well as engineering fields including such diverse problems as: the energy loss mechanisms acting in planetary rings, the slumping behavior of impact craters, landslides, the frictional resistance across (sand-filled) faults, the flow of solids in industrial, mining or agricultural applications and even proposed designs for inertially confined fusion power reactors. Yet, this behavior is poorly understood. Microstructural theories are advancing; however, inelastic, frictional contacts and multiple particle effects make progress difficult. Experimental measurements of shearing flows invariably have undesired density gradients due to gravity or centrifugal forces. Equal density liquids have been used (*e.g.*, with wax spheres in attempts to eliminate gravity induced gradients, but these have added the complication of a second phase (and its viscous damping effects). No existing experimental techniques for measuring shear and normal stresses in shearing flows can be used at solids packings as low as would exist, say, in planetary rings. Relatively low solids densities (on the order of 3% by volume solids) have been observed in the upper layers of rapid chute flows, but these have been insufficiently characterized to be useful for checking new theories or computer simulation calculations. At the high and moderate solids packings that can be achieved in earth bound shear test cells (above ~40% by volume solids) computer simulation calculations, indicate that the stress components are only moderately sensitive to such binary collision parameters as the coefficient of restitution and the coefficient of friction acting between particles. While at low solids packings the magnitude of the stress under steady shearing conditions is extremely sensitive to these collision parameters with all stress components decreasing as the energy loss in individual collisions increases.

A very low g environment such as on the Space Station offers a unique opportunity to obtain shear data without gravity induced gradients and to extend such data at least an order of magnitude lower in solids packings than can be achieved in earth bound experiments. Stresses in shearing flows at solids packings in the range from 1% to 10% solids by volume are dominated by the momentum carried by particles themselves and are very sensitive to the magnitude of the energy loss per collision. At low shear rates, nearly elastic collisions dominate and we expect a nearly Maxwellian distribution of particle velocities. At higher shear rates, higher energy losses are expected to produce a highly anisotropic distribution of deviatoric particle velocities with deviatoric velocities perpendicular to the shearing direction much lower than deviatoric velocities in a direction parallel to the shear. Experimental confirmation of these expectations is lacking.

We propose a rectilinear shear flow test to be performed in a very low g environment. One long wall in a thin rectangular box containing simple spherical grains would consist of a moving belt (probably roughened by having half-particles glued to its surface). A "floating" stress sensing area would be located in the opposite, stationary wall suspended on strain gauged elastic members. Both transverse and normal direction forces on this stress sensing element would be measured. In addition, motion pictures, through transparent side walls, would provide data on the velocity and density profiles in the sheared sample. With only one moving wall on the test cell, a particle recirculation loop would need to be provided. If desired, a second test cell could be included on the return side of the belt simultaneously measuring stresses at a different solids packing or shear rate.

(With a test cell of this design, it may be possible to achieve results sufficiently close to steady state during the several seconds of near zero-g acceleration on the NASA KC-135 aircraft. If so, this would obviate the need to do such experiments on the Space Station.)

### 6.2.2 Grain Dynamics in Zero Gravity

The dynamics of granular materials has proved difficult to model, primarily because of the complications arising from inelastic losses, friction, packing and the effect of many grains being in contact simultaneously. One interesting limit for which it has recently been possible to construct a theory is that where the grain-grain interactions are dominated by binary collisions. The kinetic model of granular systems is similar to the kinetic theory of gases, except that collision energy losses are always present in the former and must be treated explicitly. Few granular materials on earth are describable by this limiting model, since gravity tends to collapse the grains into a high-density state where Coulombic friction effects are dominant.

The planned Space Station offers an unusual opportunity to test the kinetic grain model and to explore its predictions. Without gravity, we will be able to investigate the regime of low interparticle velocities, where an elastic description of the collision is still valid. This will allow for direct interpretation by dynamical computer simulations and comparison to the kinetic theory.

One effect predicted by the kinetic theory is the tendency for inelastic grains to cluster together away from a source of energy. For instance, if one wall of a box partially filled with grains in the absence of gravity is vibrated, the density of grains close to this wall will become small, while near the opposite (cold) wall the grain density approaches its maximum value. Correspondingly, kinetic grain models predict that grain "thermal" velocities become very small at a characteristic distance from the hot wall. Computer simulations of this situation also predict that the particle velocities should fall and that they should cluster away from the hot wall.

A basic experiment to be performed on the Space Station could examine the dynamics of spherical grains inside a clear box. Data would be obtained primarily from a film of the experiment and analyzed using techniques presently under development. Results would be compared with the predictions of the kinetic theory and computer simulations. In addition, the effect of grain rotations would be studied.

Planetary rings can be theoretically modeled using the kinetic theory of granular dynamics. We would like to use this experimental apparatus to investigate some of the parameters needed for such a model. In particular, we could study the clustering effect for realistic materials, as well as the details of individual two-body collisions.

### 6.2.3 Properties of Tenuous Fractal Aggregates

The process of aggregation of small particles to form layer clusters is an important example of a random, kinetic growth process. Very often, the structure of the clusters formed has a highly disordered and tenuous appearance, that, until recently, has defied quantitative characterization. However, application of modern concepts in statistical physics has enabled the development of a quantitative description of both the structure and the physical properties of such objects. The key element in this description is the recognition that the objects possess what is called dilation symmetry, that is, their structure is invariant in a statistical sense, to a change in length scale. Such objects are called fractals, because the scale invariance implies that the mass of the clusters is related to their size by a power law, $M \sim \mathrm{R}^D$, where the fractal dimension, $D$, is less than the dimension of space (3) and is typically not an integer.

There are two fundamentally important scientific issues concerning these aggregates that should be investigated. The first is their actual growth process. The power-law, or fractal, scaling of their mass with characteristic size has been demonstrated over roughly two decades in some systems on earth. At larger sizes, sedimentation precludes continued random aggregation. It is of fundamental interest and importance in the theories of kinetic growth to know how far the fractal scaling extends, and to determine the exact type of symmetry possessed by very large aggregates. These questions can probably only be answered in a low g environment because any attempt to make a neutrally buoyant suspension of particles will lead to great difficulty in controlling the aggregation process itself.

The second fundamentally important scientific question that must be investigated concerns the physical properties of these fractal objects. The fractal scaling of their mass with size implies that their density scales as $R^{D-3}$, and thus decreases as they grow. Therefore, these clusters are examples of a class of materials that becomes more tenuous and less stable as they grow larger. Such materials are predicted to have unique behavior in that their physical properties will scale with their size in a fashion that is completely different than that of most forms of matter. Thus an understanding and measurement of their mechanical, optical, thermal and electrical properties should lead to completely new behavior. Again, our ability to perform such measurements on earth is limited in two ways. First, sedimentation can prevent the formation of samples large enough for macroscopic measurements. Secondly, a more fundamental constraint is imposed by gravity in that it limits the ultimate size of the objects that can be formed. If scale invariance is maintained to large enough sizes, the clusters will literally collapse under their own weight. Thus a low-g environment will allow us to obtain material in a regime that has never before been achieved, much less studied. This new class of materials is bound to have some fundamentally interesting and potentially important properties.

The experiments envisaged are relatively simple and can probably be integrated with many others. A source of small particles is required — they can either be produced in space or brought up from earth. Kinetic growth is initiated and the structure and kinetics of this growth monitored. This can be conveniently done with laser light scattering techniques, although electron or optical microscopy would also be useful. When formed, the clusters would be collected and their physical properties measured. This would probably involve some simple measurements of electrical conductivity, mechanical strength and rheological behavior. The major problem would be in the extreme fragile nature of the structures, which would require fairly delicate measurements.

The knowledge gained from this work will be directly relevant to the many questions being asked about the formation and aggregation of particulate matter of astrophysical importance, such as cosmic dust. It also represents the study of a new class of materials with many potentially important properties, that cannot be formed in the gravitational environment found on earth.

### 6.2.4 Orientation of Weakly Ferroelectric Dust Grains

Low-Z elements, in particular carbon, play an important role as contaminants in structurally dense oxide and silicate matrices. Carbon becomes structurally incorporated when any oxide/silicate crystal grows in an environment that contains a finite partial pressure of $CO/CO_2$: the gaseous components form solid solutions with the refractory minerals. The solubility is small, because carbon is a structurally incompatible impurity in any dense oxide/silicate matrix. The solubility depends, however, on the grain size and imperfection: small grains which are not well crystallized (because, for instance, they condensed out a chemically complex vapor at relatively low temperatures) contain more carbon than large single crystals. Yet even traces of carbon have a pronounced effect upon certain physical and chemical properties of the mineral grains as will be briefly outlined here.

When carbon becomes structurally incorporated, it forms anion complexes, in particular $CO_2^{2-}$ and $CO^-$. One of the outstanding features of these complexes is that they are dipolar: they are electric dipoles as well as elastic dipoles. When sufficient defects of this nature are present in a given oxide/silicate grain per unit volume, they undergo ordering. The main consequence of this is that it leads to the formation of ferroelectric domains, even if the structure of the oxide or silicate is intrinsically centrosymmetric and thus unable to exhibit physical properties which require a polar axis.

The ferroelectric response of olivine has been demonstrated recently as part of an on-going research effort to understand the role of carbon and other low-Z element impurities in structurally dense minerals. From these results we deduce that small dust grains, which consist of typical ultramafic minerals such as olivine, should represent single ferroelectric domains. If so, an ensemble of freely suspended olivine grains is expected to orient in an externally applied electric field. The same is expected to hold when the grains move at a constant speed through a homogeneous magnetic field.

The fundamental interest in this phenomenon is that it may represent a mechanism by which interstellar dust grains are oriented in the galactic magnetic field. It is to be noted that olivine is probably quantitatively the most abundant silicate phase in the interstellar medium, forming either individual grains or acting as cores for composite grains. So far, there seems to be no valid concept of how interstellar dust grains can be oriented, unless they are ferromagnetic. Small iron or magnetite needles have been discussed, but it is questionable whether they are present in sufficient number to cause the observed degree of orientation. Olivine appears to fulfill the major requirements which are needed to produce oriented interstellar dust particles.

We are considering a research program for the study of the dielectric/ferroelectric properties of simulated interstellar dust grains. For ground-based experiments, in order to firmly establish the predicted ferroelectric response of fine-grained material, one would use loosely packed powders, or powders which are suspended in equal-density liquids. For a more advanced stage of the project one would set up an experiment under microgravity conditions. For this we would require a large vacuum chamber into which dust grains can be injected and studied under the influence of externally applied fields. The requirements for the chamber to conduct such an experiment are basically not different from those proposed by other interested parties for the study of freely suspended dust.

### 6.2.5 Supersonic Nozzle Beam

When a gaseous source at a pressure $P_o$ is allowed to expand into a vacuum through a hole whose diameter is much larger than the mean-free-path of the gas (corresponding to the pressure $P_o$), the random translation motion of the gas is converted to directed motion thereby isentropically cooling the gas. Temperatures down to 30 millikelvin are possible. If the gas is molecular, rotational and vibrational temperatures are also reduced, but not as much as that of the translation. The temperature may drop sufficiently rapidly during the expansion to cause condensation producing clusters of the gas atoms or molecules in the region in the nozzle where the pressure is still sufficiently high to allow three-body collisions to occur. Eventually, of course, the expansion is so thorough that no further collisions occur and the cluster distribution (and rotational and translational temperatures) are "frozen in."

This technique is very well established and is commonly used to:

1. Cool molecules so as to minimize spectral congestion in a subsequent spectroscopic analysis.
2. Create reagents with known translational energies for chemical dynamical studies.
3. Make metal cluster beams in order to investigate the properties of clusters as a function of cluster size.

The most popular current technique generates clusters by entraining metal vapor which has been generated by laser-vaporizing a metal target in a helium atmosphere which is forced through a nozzle.

There are other techniques for vaporizing metal, such as hollow cathode sputtering which can generate orders of magnitude more metal flux. The requirements in pumping speed, however, make such an experiment costly and very cumbersome.

The large pumping speeds available in space make the cluster beam experiment a candidate for the Space Station. The size of the "vacuum chamber" on the station, which may be the outside of the station, make feasible such techniques for cluster beam separation as centrifugation, which cause clusters of different mass to deviate by a small angle from one another. These small angles may be translated into large displacements if the drift length for the beam was large enough, bringing up the possibility of collecting clusters of different size, trapping them, for example, in porous oxide supports for terrestrial investigation. In this way, the catalytic, structural and spectroscopic properties of clusters of metal atoms may be investigated as a function of cluster size.

In order to provide the pumping speed demanded by a system which produces clusters at a sufficient rate so that they may be separated and collected on earth, special pumps and chambers must be constructed at a cost that would likely surpass that of performing the experiment in space.

### 6.2.6 Some Astrophysical Cluster Experiments

Two sets of specific moieties that would be essential to study with the cluster techniques described above are silicon and carbon based species. The primary reason for the interest in these apart from the serendipitous aspect of discovering a new form of carbon and silicon with unusual electric and catalytic properties is that they make up the bulk of interstellar solid material that is produced in space. These, in turn, form the nucleation centers for other species and are the material from which comets, meteorites, planets and stars are formed.

The period of interest in stellar evolution is the epoch following the H and He burning phase of a star when the heavier elements, such as carbon and silicon, are produced. As this material is ejected as atoms into a circumstellar shell, refractive particles such as $Si_nO_m$, SiC, $C_nH_m$ and "graphite" are believed to form.

The amount of each type is dictated by the amount of oxygen available relative to carbon. If oxygen dominates (the O/C ratio is greater than 1), silicon condenses out primarily as an oxide and carbon does not form particles but is tied up in the gas CO. If the oxygen to carbon ratio is less than 1, the silicon condenses out primarily as silicon carbide (SiC) and carbon particles are formed. Although there is no definite spectroscopic evidence strongly in its favor, carbon is believed to condense out as sheets of graphite on the order of 50 nm in size. There is recent, good spectroscopic evidence that a large fraction of the carbon is not in the form of graphite, but in the form of polycyclic aromatic hydrocarbons. Whether they are present as free molecules or as constituents of particles is not clear.

To date, there is no theory available that can describe how these particles are formed under the conditions prevalent in the circumstellar shell and no laboratory produced material can reproduce the spectroscopic signatures observed in detail. Thus, in addition to the other systems to be studied in microgravity particle chamber cluster experiments, silicon and carbon cluster formation experiments are extremely important as well. Naturally, in addition to characterizing the types of clusters formed, the optical properties from the ultraviolet through the infrared should also be determined. Without this type of information all that the best observatories and satellites can do is provide more uninterpretable data. Without a laboratory in which realistic samples can be produced, little progress will be made in these areas.

## 6.3 Required Capabilities of an Orbital Facility

### 6.3.1 Required Analytical Capabilities

An appropriate use of some of the space and resources allocated for particle research may include state-of-the-art surface chemical analysis capabilities and scanning electron microscopy with energy dispersed X-ray detector (EDX). These two capabilities would be routine tools for many experiments (high versatility and applicability) and should be designed in a flexible manner. They should be positioned near vacuum for high-speed pumping, and the surface analysis method should be provided with excellent UHV characteristics (proper material selection, and pumping in a constant wake). Space, weight, and power consumption should be modest, with power consumed only when doing the analysis (no pumps), possibly less than a few kilowatts when running.

Perhaps the most appropriate surface analysis method for the Space Station at the present time is the surface analysis by laser ionization (SALI) technique recently developed at SRI. This method has extreme sensitivity and is quantifiable, while being strictly surface sensitive, but useful for depth profiling as well. It also is valuable for gas analysis and studies of particle-induced desorption and evaporation from grain and material surfaces. The method is mass spectrometric, using time-of-flight mass spectrometry, and general and efficient ionization of sputtered or desorbed neutral atoms, molecules, and clusters by nonresonant laser radiation. It is reasonably likely that a commercial unit based on this method will be available before 1990, which along with an SEM instrument would alleviate the need for major special designing. It is worth noting that related uses of time-of-flight mass spectrometry are featured in two recent Soviet space probes, Halley's comet, and to Mars' moon Phobos.

Applications of SALI include, but are not limited to, the following types of experiments and characteristics: determination of mass spectra of molecules and microparticles up to weights of $10^4$ to $10^5$ amu; chemical mapping of surface composition of recovered extraterrestrial particles at a spatial resolution of 200 nm or less, to the 1% level; isotope analysis; measurements of the sticking coefficients of molecules during accretion; measurements of particle outgassing and particle and cluster fragmentation during collisions; study of the (organic) chemistry occurring on the surfaces of extraterrestrial and artificial grains; and monitoring of on-board gases.

### 6.3.2 Volume and Communications

With the exception of the molecular beam experiments, the 3 $m^3$ space discussed in some detail in Chapter 2 of this report, as well as the instrument lists compiled by the other subgroups, will suffice. For the beam experiments a nozzle that allows expansion of gases into space through an appropriate port and a manipulator that may sample the beam outside the station would be needed. In addition, we suggest the instrumental compliment discussed above.

It was also felt that it was crucial that the experimental design in the Station be such to allow the principle investigators to communicate in real time with the experimenters on board so as to be able to make follow-up decisions regarding subsequent phases of an experiment based on initial results.